

Isocitric lactone, bis(trimethylsilyl)-

Other names:	Isocitric lactone acid, bis(trimethylsilyl) ester Isocitric acid lactone, bis(trimethylsilyl) ester Lactoisocitric acid, TMS Isocitric acid lactone, 2tms derivative
Inchi:	InChI=1S/C12H22O6Si2/c1-19(2,3)17-11(14)8-7-9(13)16-10(8)12(15)18-20(4,5)6/h8,10H
InchiKey:	IBEFDHMMOJYHKQ-UHFFFAOYSA-N
Formula:	C12H22O6Si2
SMILES:	<chem>C[Si](C)(C)OC(=O)C1CC(=O)OC1C(=O)O[Si](C)(C)C</chem>
Mol. weight [g/mol]:	318.47
CAS:	65143-62-6

Physical Properties

Property code	Value	Unit	Source
log10ws	2.70		Crippen Method
logp	1.674		Crippen Method
rinpol	1710.40		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65143626&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/17-249-7/Isocitric-lactone-bis-trimethylsilyl.pdf>

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